The Use of X-Ray Thomson Scattering for The Study of Warm Dense Matter

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Talk outline

- Physical properties of Warm Dense Matter (WDM)
- Overview of X-ray Thomson Scattering (XRTS)
  - Theoretical description
  - Spectral features
- Examples of XRTS experiments and EOS measurements
  - High power laser facilities
  - Free electron lasers
  - Spatially resolved XRTS measurements
  - Combination with other diagnostics (VISAR, SOP, radiography, etc.)
- Conclusion
Warm Dense Matter
Warm Dense Matter (WDM) conditions

- WDM is an intermediate state between solids and plasmas:
  - Temperature: 1 – 100 eV
  - Density: ~ 1 g/cm³ (solid densities)
- Ions are strongly coupled and fluid-like, do not exhibit long-range order. The electrons are fully or partially degenerate
  => quantum effects become important in WDM
- Planar shocks in laser-plasmas (solid-to-plasma transitions) or as an intermediate state during ICF implosions
- Astrophysical objects: interiors of giant planets, brown dwarfs, white dwarfs, low-mass stars, crusts of old stars, etc.
- The equation of state (EOS) in the WDM regime is largely unknown
Physical parameters of WDM

- **Degenerate matter**: thermal energy of the particles smaller than or comparable to the Fermi energy (WDM fully or partially degenerate)

  - **Fermi energy**: 
    \[ E_F = \frac{\pi^2 \hbar^2}{2m_e} \left( \frac{3n_e}{\pi} \right)^{2/3} \]

  - **Degeneracy parameter**: 
    \[ \theta = \frac{k_B T}{E_F} \]

  - **Wigner-Seitz parameter**: 
    \[ r_s = \frac{d}{a_B} \]  
    
    When \( \theta < 1 \) most electrons populate the states within the Fermi sea and cannot further reduce the distance between them due to the Pauli exclusion principle.

    \[ d = (3/(4n_e))^{1/3} \] = inter-particle spacing

    \[ a_B = 5.29 \times 10^{-11} \text{ m} = \text{Bohr radius} \]

Metals: \( r_s = 2 - 6 \)
**Physical parameters of WDM**

- **Strongly coupled plasmas:** Coulomb interactions between the particles determine the physical properties of the system (ideal gas equation of state invalid)

- **Coupling parameter:**
  \[ \Gamma_{\alpha,\beta} = \frac{Z_{\alpha}Z_{\beta}e^2}{4\pi\varepsilon_0 a_{\alpha,\beta}k_BT} \]

  (ratio of Coulomb & thermal energy)

  \( \Rightarrow \) strongly coupled plasma for \( \Gamma_{ii} > 1 \)
X-ray Thomson Scattering
X-ray Thomson scattering (XRTS) overview

- Scattering cross-section and power depend on dynamic structure factor:
  \[
  \frac{d^2 \sigma}{d\Omega d\omega} = \sigma_T \frac{k_1}{k_0} S(k, \omega)
  \]

- Dynamic structure factor [Chihara 1987, 2000]:
  \[
  S_{ee}^{tot}(k, \omega) = |f_1(k) + q(k)|^2 S_{ii}(k, \omega) + Z_f S_{ee}^0(k, \omega) + Z_c \int \tilde{S}_{ee}(k, \omega - \omega') S_s(k, \omega') d\omega'
  \]

- The electron-electron structure factor is linked to the dielectric function through the fluctuation-dissipation theorem [Kubo, 1957]:
  \[
  S_{ee}^0(k, \omega) = -\frac{\hbar}{(1 - e^{-\hbar\omega/(k_B T_e)})} \frac{\epsilon_0 k^2}{\pi e^2 n_e} \text{Im} \left[ \frac{1}{\varepsilon(k, \omega)} \right]
  \]

References:
X-ray Thomson scattering overview

- Scattering vector: \( k = \left( \frac{4\pi}{\lambda_0} \right) \sin(\theta/2) \)

- Plasma screening length:
  \[
  \lambda_s \sim \lambda_{TF} = \frac{2\varepsilon_0 E_F}{3n_e e^2}
  \]
  (Thomas-Fermi length)

- Scattering parameter: \( \alpha = 1/k\lambda_s \)

- Scattering parameter:
  \( \alpha > 1 \) collective scattering
  (off plasmons)

  \( \alpha < 1 \) non-collective scattering
  (off individual electrons)

S. H. Glenzer and R. Redmer, Rev. Mod. Phys. 81, 1625 (2009)
X-ray Thomson scattering overview

- X-ray scattering from warm dense deuterium at different conditions and geometries:

**Rayleigh peak**: elastic scattering (bound electrons)

**Compton peak**: inelastic scattering (free/metallic electrons)
Non-collective X-ray Thomson scattering

- The shape of the free electron feature (Compton peak at $E_C$) reflects the velocity distribution of the free electrons and gives electron temperature $T_e \Rightarrow$ Doppler broadening:

\[
\Delta \omega = -\frac{\hbar^2 k^2}{2m_e} \pm k.v
\]

\[
E_C = \frac{\hbar^2 k^2}{2m_e}
\]

- **Velocity distribution** (Maxwell-Boltzmann or Fermi-Dirac) can be fitted to the inelastic peak:

\[
f(v_x)dv_x = \int_0^{\pi/2} n\left(\frac{v_x}{\cos \beta}\right) \frac{v_x^2}{\cos^2 \beta} \tan \beta d\beta
\]

- The shape of the peak/electron distribution can be calculated using the finite temperature random phase approximation (RPA):

\[
\varepsilon(k, \omega) = 1 - \frac{e^2}{\hbar\varepsilon_0 k^2} \int \frac{f(p + \hbar k/2) - f(p - \hbar k/2)}{k.p/m_e - \omega - iv} \frac{2d^3p}{2\pi \hbar^3}
\]

S. H. Glenzer and R. Redmer, Rev. Mod. Phys. 81, 1625 (2009)
Collective X-ray Thomson scattering

- Following Bohm-Gross relation, the down and up shift of the plasmon peaks depend on the plasma frequency and thus provide an accurate measure of electron density $n_e$:

$$\omega^2 = \omega_p^2 + 3k^2\nu_{th}^2(1 + 0.088n_e\Lambda_n^3) + \left(\frac{\hbar k^2}{2m_e}\right)^2$$

$$\omega_p = \sqrt{\frac{n_e e^2}{\varepsilon_0 m_e}}$$

- Imaginary part of the dielectric function determines the Landau damping of the plasmon waves which provides a measure of the electron temperature $T_e$:

$$\delta\omega \approx -\frac{i}{2}\sqrt{\frac{\pi}{2}} \frac{\omega_p}{(k\lambda_{De})^3} \exp\left[-\frac{1}{2(k\lambda_{De})^2}\right]$$

$$\lambda_{De} = \sqrt{\frac{\varepsilon_0 k_B T_e}{e^2 n_e}}$$

- An alternative temperature measurement in the collective regime is possible from the relative ratio of the Stokes and anti-Stokes components in the inelastic scattering spectrum using the detailed balance relation:

$$\frac{S(k, \omega)}{S(-k, -\omega)} = e^{-\frac{\hbar\omega}{k_B T_e}}$$

S. H. Glenzer and R. Redmer, Rev. Mod. Phys. 81, 1625 (2009)
X-ray Thomson scattering overview

- Determine the elements of EOS from features of scattering spectra:
  - Electron temperature ($T_e$) from width of the inelastic peak (or detailed balance)
  - Electron density ($n_e$) from downshift of a plasmon peak (collective scattering)
  - Ion temperature ($T_i$) from elastic scattering strength
  - Average ionization state ($Z$) from intensity ratio of the Rayleigh and Compton peaks
  - Atomic structure from bound-free tail contribution

- G. Gregori (contributions from C. Fortmann, D. Gericke, et al.) has created an easy to use XRS analysis code to extract information out of XRTS data by fitting theoretical curves to the spectral profiles

- Alternative analysis codes have now also started appearing, e.g., Souza et al., D. A. Chapman, etc.
  
Experiments
First XRTS measurements of radiatively heated Be at Omega

- Non-collective:
  - Ti He-alpha @ 4.75 keV
  - $\theta_B = 125^\circ$, $\alpha = 0.4$
  - $T_e = 53$ eV $\pm$ 20%
  - $n_e = 3.3 \times 10^{23}$ cm$^{-3}$ (from $\rho$ and $Z$)

- Collective:
  - Cl Ly-alpha @ 2.96 keV
  - $\theta_B = 40^\circ$, $\alpha = 1.6$
  - $T_e = 12$ eV
  - $n_e = 3 \times 10^{23}$ cm$^{-3}$
  - plasmon shift $\omega_p \approx 20$ eV


Other notable experimental XRTS work

Notable publications:

- S. White et al., HEDP 9, 573-577 (2013)

... and many more ...
Ultrafast non-equilibrium XRTS in warm dense hydrogen using the FLASH free electron laser as an x-ray probe

- Experiment carried out at DESY facility, Germany
- X-ray pump/probe: FLASH beam @ 91.8 eV
- 5 Hz rep. rate, ~40 fs pulse duration, I~8x10^{13} Wcm^{-2}
- Fluctuation-dissipation theorem not valid here
- New non-equilibrium theory was used to reanalyze the spectra showing a strong temporal dependence of the spectral shapes => improved fit

Collective XRTS:
- \( T_e = 13 \text{ eV} \)
- \( n_e = 2.8 \times 10^{20} \text{ cm}^{-3} \)

Observation of continuum depression in WDM using XRTS

- Experiment at Omega laser, U. of Rochester
- $n_e > 10^{24}$ cm$^{-3}$, $Z_C = 4$, $P \approx 50$ Mbar, $T_e < T_F$
- Non-collective XRTS
Strong ion-ion correlations in shock-compressed Al

- Experiment at Omega laser, U. of Rochester

Complex ion structure in liquid carbon at 100 GPa

- Experiment at GSI, Germany
- Shock and particle velocity measured independently using streaked optical pyrometry and multiframe shadowgraphy
- Complex structure of Carbon observed

Combined XRTS and VISAR measurements of isochorically heated Al at MEC station (LCLS)

- Al isochorically heated by x-ray beam
- Combined collective and non-collective XRTS provided accurate measurement of $n_e$
- Laser beam was used to drive a shock wave in the Al sample
- VISAR was used to measure shock velocity and provide shock pressure in Al

$n_e = 1.8 \times 10^{23} \pm 5\%$

Combined XRTS and x-ray radiography measurements on dense shock-compressed Boron

- Experiment at Titan laser, LLNL
- Collective and non-collective XRTS
- X-ray radiography

Imaging X-ray Thomson Spectrometer (IXTS)

- A novel diagnostic particularly suitable for shock-release experiments developed by LANL and the University of Michigan to operate in a standard TIM setup
- Toroidal Ge crystal used to provide spatial and spectral resolution on the same image
- Crystal and detector setup modified to fit into standard TIM ports used on Omega and NIF
  - Spatial resolution = 25 µm (<50 µm)
  - Spectral resolution = 4-5 eV
  - Two possible crystal configurations:
    - Zn He-alpha line at 9 keV
    - Ni He-alpha line at 7.8 keV

E. J. Gamboa et al., JINST 6, P04004 (2011)
Advantage of using highly reflective toroidal crystals

- High throughput
- Imaging localizes noise sources
- Free from astigmatism at low $\theta_B$
- No source broadening

- Crystal: Ge(220) with $R_v = 10$ cm and $R_h = 92$ cm
- Detector: Princeton Instruments PI-MTE deep-depletion x-ray CCD

Horizontal and vertical foci:

$$f_h = \frac{1}{2} R_h \sin \theta_B$$
$$f_v = \frac{R_v}{2 \sin \theta_B}$$

Johann spectrometer geometry:

$$d_{cd} = R_h \sin \theta_B$$
$$d_{sc} = \frac{R_v}{2 \sin \theta_B} \frac{M + 1}{M}$$

Magnification:

$$M = \frac{d_{cd}}{d_{sc}} \approx 2$$

Lens maker’s formula:

$$\frac{1}{d_{sc}} + \frac{1}{d_{cd}} = \frac{1}{f_v}$$
First spatially resolved XRTS measurements at Omega


IXTS spatially resolves scattering signals from different parts of the shocked carbon foam sample.
First spatially resolved XRTS measurements at Omega

Scattering signals from different parts of the shocked carbon foam sample.

Invited talk by Eliseo Gamboa (SLAC National Accelerator Laboratory):

GI2.00006: Free-electron laser measurements of plasmons in warm dense matter: 12:00–12:30 PM

Tuesday, October 28, 2014

Session GI2: Fundamental High Energy Density Physics: 9:30 AM–12:30 PM

Room: Bissonet

Full EOS measurement using combination of XRTS, VISAR, SOP and x-ray radiography diagnostics at Omega

\[ \theta_{\text{scattering}} = 95 - 100^\circ \]

XRTS used to determine temperature of shock-released C

Temperature, pressure, density and ionization ($n_e$) extracted from experimental data:

- Temperature measurement obtained from spatially resolved non-collective XRTS using Ni He-alpha line and the IXTS diagnostic @ 7.8 keV

- XRTS measurement constrained by independent density measurement from radiography

\[ \alpha = 0.3 - 0.35 \]

Complementary radiography and VISAR/SOP measurements complete the full EOS determination

- Mass density determined from x-ray transmission radiography @ 5 keV (V He-α)
- The density measurement was also used to constrain the XRTS fitting analysis
- VISAR and SOP used to obtain pressure from shock velocity measurement:

$$P_{\text{release}} = \rho_0 u_s u_p$$

$$u_s = 1.20274 \cdot u_p + 0.507$$


Transmission ~ 0.12, corresponding to C density of 2.8 g/cm³

Comparison with EOS models: SESAME and QMD

- Experimental measurement compared to SESAME EOS tables and QMD simulations:

Summary and conclusions

- Warm dense matter (WDM) is a difficult state to describe theoretically
  - Applications in ICF, planetary science, materials and theoretical physics
- X-ray Thomson scattering (XRTS) provides accurate and non-invasive measurement of thermodynamic state and structure of WDM
  - Accurate theoretical description is very important for calculating fits to experimental data used to extract $n_e$, $T_e$, $Z$, structure, etc.
  - Non-equilibrium scattering theory is being developed for fs time scales
- Spatially resolved XRTS now demonstrated providing improved measurements
- Additional independent measurements used to constrain XRTS
  - Radiography for direct density measurement
  - VISAR for shock velocity and pressure measurements
  - SOP for temperature measurements, shock velocity, etc.
Thank you!
Any questions?

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(ELI Beamlines, Czech Republic, from Jan 2015)